

Docket No. 1073.060
U.S. Serial No. 09/595,096

REMARKS

Claims 1-30 were originally filed with the application on June 15, 2000, and are currently pending.

Rejections Under 35 U.S.C. § 101

Non-Statutory Subject Matter

Claims 1-20 are rejected under 35 U.S.C. § 101 on the grounds that the claimed invention is directed to non-statutory subject matter. The rejection is traversed.

The specification is now amended to include material from a relevant publication by a leader in the molecular docking field, and sets forth the practical applications of molecular docking procedures, such as those of the claims, in rational drug design. As the material was incorporated by reference in the application as filed, on page 20, lines 24-28, no new matter has been added to the application. The Background section of the specification as amended now begins:

"Prediction of small molecule binding modes to macromolecules of known three-dimensional structure is a problem of paramount importance in rational drug design (the "docking" problem). . . Protein binding sites exhibit highly selective recognition of small organic molecules, in that evolution has equipped them with a complex three-dimensional "lock" into which only specific "keys" will fit. This has been exploited by medicinal chemists in the design of molecules to selectively augment or retard biochemical pathways and so exhibit a clinical effect. X-ray crystallography has revealed the structure of a significant number of these binding sites. It would be advantageous in attempting the computer-aided design of therapeutic molecules to be able to predict and to explain the binding mode of novel chemical entities (the "docking" problem) when the active site geometry is known." (Jones *et al.*, *J. Mol. Bio.*, 267, pg. 727 (1997))

As noted in the Office action, MPEP 2106(IV)(B)(2)(b)(ii) states that a statutory process must be limited to a practical application in the technological arts, and, further, that the method must produce "a concrete, tangible and useful result." The Office action asserts that the claims do not recite a result of any kind such that the claimed method steps accomplish a practical application. Applicants respectfully disagree. The concrete, tangible and useful result produced by the methods and systems of the claims is the three-dimensional structure of the ligand-receptor complex, specifically the geometry of the docked compound in the active site. This type of structure is utilized extensively in designing pharmaceutical compounds having a therapeutic effect, as described in the passage above. Accordingly, applicants submit that the claimed

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invention does produce a concrete, tangible and useful result, and so, is drawn to statutory subject matter. It is believed that the rejection is hereby overcome.

Lack of Utility

Claims 1-30 are rejected under 35 U.S.C. § 101 as lacking patentable utility. Applicants submit that because the invention produces the concrete, tangible and useful results as described in the amendment to the specification presented above, it has the "practical utility" and "real-world" value required for patentable utility (MPEP §2107.01(I), quoting *Nelson v. Bowler*, 626 F.2d 853, 856, 206 USPQ 881, 883 (CCPA 1980)). The invention's function as a tool for use in drug discovery programs provides real-world value, as the structures obtained from practice of the invention are valuable, and in many cases, essential, to rational drug design. Further, this function is analogous that of the research tools, including "gas chromatographs, screening assays, and nucleotide sequencing techniques," identified in the same section of the MPEP as having "a clear, specific and unquestionable utility". Therefore, claims 1-30 do not lack patentable utility. It is believed that the rejection is overcome.

Rejections Under 35 U.S.C. § 112:

Claims 1-30 are rejected under 35 U.S.C. § 112, second paragraph, as being indefinite. Specific issues are addressed below in the order in which they were raised in the Office Action.

Regarding generating conformations *with* a search: Claims 1, 11, and 21 are now amended to recite "performing a pre-docking conformation search and generating multiple solution conformations of the ligand therefrom". Applicant submits that the amendment clarifies that the multiple solution conformations are generated using the search.

Regarding whether the step of creating a database is intended to precede the step of generating multiple solution conformations of the ligand: Claims 2, 12, and 21 are amended to recite "additionally comprising, after performing the pre-docking conformational search and generating multiple solution conformations" in order to clarify that the step of generally creating a data base and storing the data base occurs after the searching and generation step of the parent claims.

Regarding whether the generation step of claims 4, 14 and 24 is intended to replace the generation step of the parent claim: Claims 4, 14, and 24 are amended to recite "performing the pre-docking conformational search and generating multiple solution conformations of the ligand"

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in order to clarify that the generation step of the dependent claims replaces the generation step of the parent claim.

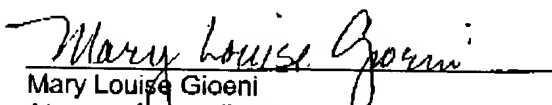
Regarding the language "in solution" in claims 1, 11, and 21, the claims are now amended to recite "generating multiple solution conformations" in order to clarify that applicant intends computer-generated conformations.

Finally, the term "molecule": Claims 4 and 7 are amended by replacing "molecule" with "ligand".

Applicant submits that these claim amendments clarify the claimed invention such that the claims are not indefinite. It is believed that the rejection is hereby overcome.

In view of the above amendments and remarks, applicants respectfully request allowance of all claims pending herein.

Respectfully submitted,


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Dated: September 24, 2003

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